Impact of interfacial charge transfer on the performance of Pd/C catalysts

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ABSTRACT BODY:
Abstract: Carbon materials are typically considered to be inert catalyst supports. This assumption implies that carbon-supported catalysts are free of metal-support interactions. However, optoelectronic applications for nanocarbons demonstrate that their electronic properties can be tailored by varying their nanoscale structure and functionalization. This information suggests that the inertness of these materials for catalytic applications should be reconsidered as nanocarbons may be candidates for electronic metal-support interactions (EMSI).

In this work, we successfully decreased the structural complexity of carbon scaffolds and controlled their graphitization and surface functionalization. This approach enabled a detailed characterization of EMSI effects on Pd nanoparticles decorating these supports. Changes in selectivity for the hydrogenation of α,β-unsaturated aldehydes were observed when varying the support properties. The trends were free of artefacts such as differences in particle size, metal loading, and mass transfer effects. Detailed characterization of the catalysts using synchrotron based X-ray photoelectron spectroscopy and aberration corrected transmission electron microscopy confirmed the presence of electronic interactions between the Pd nanoparticles and carbon surface. Correlations were established between the extent of interfacial charge transfer, support properties, and catalyst selectivity. These experimental results were also confirmed using density functional theory calculations, providing stronger evidence for the presence of EMSI in Pd/C catalysts.

Our work demonstrates how the properties of carbon materials can influence the electronic structure of the supported metal active phase and thereby impact their catalytic performance. This study provides deeper insights into the tunability of EMSI effects and opens new avenues for the rational design of carbon-supported catalysts.
(No Image Selected)